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Nonparabolicities and negative hole masses in quantum wells

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Abstract. It is shown that negative effective masses corresponding to the in-plane motion of holes in the fourth group and zinc blend heterostructure quantum wells which are usually attributed to the nonparabolicities caused by the repulsion and/or anticrossing of heavy and light hole subbands results in to the competition of two factors: the warping of the bulk energy spectrum and the phase shift of the size-quantized momentum due to heavy-light hole mixing.

Since the early studies of semiconductor heterostructures the problem of quantum well energy spectrum calculations was of prime importance. While the conduction size-quantized subbands can be easily described and interpreted within the framework of ordinary single-band quantum mechanics with all the problems lying in the determination of effective boundary conditions for envelopes the valence band subbands are usually treated by means of numerical methods because of there complex structure. The results of such numerical simulations widely present in modern textbooks demonstrate strong nonparabolicities of energy spectrum corresponding to the in-plane hole motion which are commonly associated with heavy-light hole subbands anticrossing. A common feature of the in-plane energy spectrum is the existence of the subbands with negative hole effective masses. The mass sign change could be treated in principal as a result of heavy-light hole subbands repulsion. However detailed study of energy dispersion curves for a number of structure parameters shows that it is not necessarily the case because the value of negative hole effective mass and its existence does not directly depend on the heavy-light hole subbands separation. In the present paper we investigate the origin of hole effective mass sign inversion. It is shown that apart from the heavy-light hole anticrossing two important mechanisms take place: the warping of heavy hole bands which is present already in the bulk and the in-plane quasimomentum dependent phase shift of the quantized quasimomentum due to heavy-light hole mixing.

We start from the standard Luttinger Hamiltonian:

$$H = \begin{pmatrix} P+Q & L & M & 0 \\ L^* & P-Q & 0 & M \\ M^* & 0 & P-Q & -L \\ 0 & M^* & -L^* & P+Q \end{pmatrix}, \tag{1}$$

where:

$$\begin{aligned} P &= \frac{\gamma_1}{2m_0}(k_x^2+k_y^2+k_z^2), \\ Q &= \frac{\gamma_2}{2m_0}(k_x^2+k_y^2-2k_z^2), \\ L &= -\frac{i\sqrt{3}\gamma_3}{m_0}(k_x-ik_k)k_z, \end{aligned}$$

$$M = \frac{\sqrt{3}\gamma_2}{2m_0}(k_x^2 - k_y^2) - i\frac{\sqrt{3}\gamma_3}{m_0}k_x k_y.$$

Energy spectrum of the Hamiltonian possesses two double-degenerate branches of heavy and light holes:

$$E = P \mp \sqrt{Q^2 + |L|^2 + |M|^2}. \tag{2}$$

A qualitative picture of level anticrossing can be obtained if one averages the Hamiltonian (1) over the size-quantized subband wave function localized in the well [1]. Odd terms in respect to k_z (L-terms) vanishes after this procedure. The retaining Hamiltonian can be block-diagonalized and the resulting spectrum demonstrate anticrossing of heavy and light hole subbands.

Note however that the M-term contribution to energy spectrum is of the 4-th order in respect to the in-plane quasimomentum $k_\perp$. Hence anticrossing described by the M-term in the Hamiltonian has nothing in common with possible effective mass sign change which is to be described by quadratic in $k_\perp$ terms.

Let us turn to the bulk spectrum (2). A qualitative understanding of the peculiarities of energy spectrum in size-quantized structures can be obtained if we simply take k_z equal constant k_{zn}.

To estimate the effective masses we can omit M-term in the equation (2) and expand energy expression over $k_\perp^2$ up to the first order. It is useful to present the result both in terms of Luttinger and A, B, C parameters:

$$\begin{aligned} E_{h,l} &\approx (\gamma_1 \mp 2\gamma_2)\frac{\hbar^2 k_{zn}^2}{2m_0} + \left[\gamma_1 \pm \gamma_2 \mp \frac{3\gamma_3^2}{\gamma_2}\right]\frac{\hbar^2 k_\perp^2}{2m_0} \\ &= (A \mp B)\frac{\hbar^2 k_{zn}^2}{2m_0} + \left[A \mp B \mp \frac{C^2}{2B}\right]\frac{\hbar^2 k_\perp^2}{2m_0}. \end{aligned} \tag{3}$$

The term with the coefficient γ_3 in (3) arises from the L-term in the Hamiltonian which is responsible for warping of bulk energy spectrum in the plane containing quantized z-axes. (Note that M-term also describes warping but in xy-plane dosn't contain quantized axis). It immediately follows from (3) that a negative contribution to heavy hole subband effective mass exists always. This contribution presents if and only if warping is taken into account and is absent in the so-called spherical approximation [2, 3].

For all most popular semiconductors such as $GaAs$ ($\gamma_1 = 7.65$, $\gamma_2 = 2.41$, $\gamma_3 = 3.28$), Si ($\gamma_1 = 4.22$, $\gamma_2 = 0.39$, $\gamma_3 = 1.44$), Ge ($\gamma_1 = 13.35$, $\gamma_2 = 4.25$, $\gamma_3 = 5.69$) (see e.g. [4]) this contribution exceeds the first two terms in square brackets and the coefficient at $k_\perp^2$ in (3) is negative. Because warping is the characteristic of bulk energy spectrum the coefficient at $k_\perp^2$ in (3) can be considered as a bare effective mass for the in-plane motion in quantum wells which is negative for heavy holes. In the spherical approximation ($\gamma_3 = \gamma_2$) the coefficient at $k_\perp$ in (3) is positive in common semiconductors.

In the expression (3) we don't yet take into account the dependence of size-quantized momentum k_{zn} upon $k_\perp$ which results from heavy-light hole mixing at semiconductor heterointerface. At small $k_\perp$ we can write

$$k_{zn} = k_{zn0} + \alpha L k_\perp^2, \tag{4}$$

where L is the quantum well width. It is natural to interpret the second term in (4) as a phase shift due to heavy-light hole mixing at semiconductor heterointerface. Collecting the contributions from both (3) and (4) we obtain for the in-plane effective masses the following expressions

$$\frac{1}{m_{h\perp}} = \gamma_1 + \gamma_2 - \frac{3\gamma_3^2}{\gamma_2} + 2\alpha_{hn}(\gamma_1 - 2\gamma_2)k_{zn0}L, \tag{5}$$

$$\frac{1}{m_{l\perp}} = \gamma_1 - \gamma_2 + \frac{3\gamma_3^2}{\gamma_2} + 2\alpha_{ln}(\gamma_1 + 2\gamma_2)k_{zn0}L. \tag{6}$$

If $\alpha > 0$ then the phase shift (last term in the expressions (5), (6)) pushes the effective mass to positive values. To calculate α one should find the general solution of the Schrödinger equation with the Hamiltonian (1) satisfying proper boundary conditions. Widely accepted choice of boundary conditions for semiconductor heterostructures assumes continuity of the wave functions

$$\hat{\psi}(z_{0-}) = \hat{\psi}(z_{0+}) \tag{7}$$

and the "currents"

$$\hat{j}_- \hat{\psi}(z_{0-}) = \hat{j}_+ \hat{\psi}(z_{0+}) \tag{8}$$

at the heterointerface located at z_0, where $\hat{j}$ is the "current" operator which can be obtained by the integration of the Hamiltonian over the heterointerface [2]. The problem can be studied analytically in the case of infinitely high barriers (a box or a semiconductor film). For the box boundary conditions reduces to

$$\hat{\psi}(0) = \hat{\psi}(L) = 0. \tag{9}$$

For the first time this approach was realized in [5] where however because of sign drop an erroneous conclusion was made that the highest hole subbands in *Si* and *Ge* films possesses negative (electron-like) masses. In the case of infinite barriers for the first heavy hole subband we obtain

$$\alpha_{h1} = \frac{3}{2\pi^2}\frac{\gamma_3^2}{\gamma_2^2}\sqrt{\frac{\gamma_1 + 2\gamma_2}{\gamma_1 - 2\gamma_2}}\frac{1 + \cos\theta}{\sin\theta}, \tag{10}$$

where:

$$\theta = k_{zh0}\sqrt{\frac{m_l}{m_h}}L = \pi\sqrt{\frac{\gamma_1 - 2\gamma_2}{\gamma_1 + 2\gamma_2}}. \tag{11}$$

From (5), (10) it follows that for common semiconductors hole effective mass for the topmost subband is positive. However if one instead of (7), (8) takes the generalized boundary conditions [6, 7, 8] describing heavy-light hole mixing already at normal incidence ($k_\perp = 0$) the coefficient α can be depressed and the effective mass can become negative. Numerical diagonalization of matrix 16×16 resulting from the conditions (7), (8) shows that at lower barrier the $k_\perp$—independent part of quantized quasimomentum decreases. In the expression (11) it corresponds to the reduction of k_{zho} resulting in the reduction of the denominator containing sin-function in (10). So for quantum wells with finite barrier height the tendency to the negative masses in the topmost subband is further supressed. For higher subbands the expression for α is similar to (10) however its sign oscillates with subband number becuase of the variation of the sin sign as k_{zn} changes over π/L. Another source of α sign variation is the reduction of barrier height. If k_{zn} for heigher barrier slighly exceeds π/L then for smaller barrier it will pass below the π/L and the sign of α will be changed. Hence the subband curvature for different barrier height can be dufferent.

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